

tert-Butyl nitrite

540-80-7 | DTXSID10202316

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

## Model Results

**Predicted value:** 2.26

**Global applicability domain:** Inside

**Local applicability domain index:** 9.92e-01

**Confidence level:** 7.68e-01

## Nearest Neighbors from the Training Set

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1-Pentene

**Measured:** 1.93

**Predicted:** 2.26

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Diethyl ether

**Measured:** 2.19

**Predicted:** 2.18

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1,1-Dichloroethane

**Measured:** 2.41

**Predicted:** 2.18

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1-Chloropropane

**Measured:** 2.24

**Predicted:** 2.18

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Methyl tert-butyl ether

**Measured:** 2.58

**Predicted:** 2.53